LOCALIZATION OF ELECTRONIC WAVE FUNCTIONS ON QUASIPERIODIC LATTICES

Thomas Rieth, Uwe Grimm, Michael Schreiber
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

We study electronic eigenstates on quasiperiodic lattices using a tight-binding Hamiltonian in the vertex model. In particular, the two-dimensional Penrose tiling and the three-dimensional icosahedral Ammann-Kramer tiling are considered. Our main interest concerns the decay form and the self-similarity of the electronic wave functions, which we compute numerically for periodic approximants of the perfect quasiperiodic structure. In order to investigate the suggested power-law localization of states, we calculate their participation numbers and structural entropy. We also perform a multifractal analysis of the eigenstates by standard box-counting methods. Our results indicate a rather different behaviour of the two- and the three-dimensional systems. Whereas the eigenstates on the Penrose tiling typically show power-law localization, this was not observed for the icosahedral tiling.

1 Introduction

There are, at least, three popular, yet apparently unrelated, approaches aimed at a better understanding of the peculiar transport properties of quasicrystals. Among those is the Hume-Rothery picture, which gives a plausible explanation for the presence of the pseudo-gap in the electronic density of states at the Fermi level. Another approach considers quasicrystals as a conglomerate or as an hierarchical arrangement of clusters. Here, we follow a third approach by investigating localization effects of electronic states caused by quasiperiodicity. For this purpose, we consider tight-binding Hamiltonians on periodic approximants of the two-dimensional Penrose and the icosahedral Ammann-Kramer-Neri (AKN) tiling and perform a statistical analysis of their eigenstates.

2 Tight-binding model

In the vertex model, an atomic orbital $|j\rangle$ is placed at every vertex j of the quasiperiodic tiling, and the Hamiltonian has the form

$$\mathcal{H} \;=\; \sum_{j,k=1}^{N} |j\rangle\, t_{jk}\, \langle k| \;+\; \sum_{j=1}^{N} |j\rangle\, V_j\, \langle j| \tag{1}$$

where the hopping amplitudes are $t_{jk} = 1$ for vertices j and k connected by a bond, and $t_{jk} = 0$ otherwise. The on-site potentials are chosen as $V_j = 0$, hence

the spectrum of $\mathcal{H}$ is symmetric around $E = 0$. A simple characterization of an eigenstate $|\psi\rangle$ of $\mathcal{H}$ is given by the *participation number* P, defined by

$$P^{-1} \;=\; \sum_{j=1}^{N} \psi_j^{\,4}\,, \qquad |\psi\rangle \;=\; \sum_{j=1}^{N} \psi_j\,|j\rangle\,, \tag{2}$$

which can be interpreted as an estimate of the number of vertices which carry a significant part of the wave function amplitude. With increasing system size N, the participation number grows linearly with N for *extended* states, while it approaches a constant for *localized* states.

Another interesting quantity is the so-called *structural entropy* [1]

$$S_{\rm str} \;=\; -\sum_{j=1}^{N} |\psi_j|^2\,\ln|\psi_j|^2 \;-\; \ln P\,, \tag{3}$$

the first term being the familiar Shannon entropy. However, while plots of $S_{\rm str}$ against the *participation ratio* $p = P/N$ may look different for various decay forms of the wave functions, this need not be the case and one has to be very careful if one intends to extract conclusive information on the decay form.

In the box-counting method, the system is divided into boxes of linear size δ. We denote the probability amplitude in the kth box by $\mu_k(\delta)$. Its normalized qth moment $\mu_k(q,\delta)$ constitutes a measure. From this, one obtains the Lipshitz-Hölder exponent or singularity strength α of an eigenstate and the corresponding fractal dimension f by

$$\alpha(q) \;=\; \lim_{\delta\to 0} \textstyle\sum_k\, \mu_k(q,\delta)\,\ln\mu_k(1,\delta)/\ln\delta\,, \tag{4}$$

$$f(q) \;=\; \lim_{\delta\to 0} \textstyle\sum_k\, \mu_k(q,\delta)\,\ln\mu_k(q,\delta)/\ln\delta\,, \tag{5}$$

yielding the characteristic singularity spectrum $f(\alpha)$ in a parametric representation.

3 Results: Penrose and Ammann-Kramer-Neri tiling

For the Penrose tiling, roughly 10% of the spectrum consists of degenerate states in the band center ($E = 0$),[2] separated from the rest of the band by a finite energy gap. The degenerate eigenstates are combinations of strictly localized (confined) states.[2,3] For the AKN tiling, one also observes a small number of degenerate states in the band center, but there is no indication of an energy gap in the spectrum.[1]

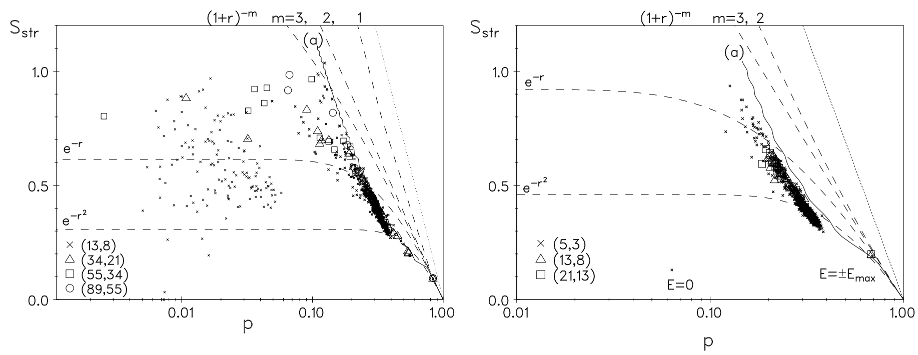


Figure 1: Structural entropy S_{str} [Eq. (3)] as function of the participation ratio $p = P/N$ [Eq. (2)] for periodic approximants of the Penrose (left) and the AKN (right) tiling, compared with the dependence (dashed lines) of wave functions of different shapes.

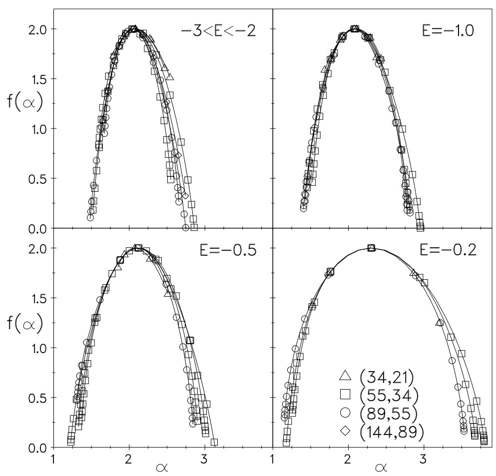
In Ref. 4, the scaling behaviour of the participation number was discussed for the two examples. For the Penrose case, a power-law behaviour $P \sim N^{\beta}$ was found, with an exponent β that is smaller than one, decreasing towards the band center. This indicates that the envelope of the eigenfunction shows a power-law decay. A closer investigation reveals that the state at the band edge is in fact extended.[1] The situation is very different for the AKN tiling: here the participation number of states close to the band edge scales with $\beta < 1$, hinting at a power-law decay, while β quickly grows to $\beta \approx 1$ as one moves towards the band center, compatible with the presence of extended states.[1,4]

Fig. 1 clearly shows a strong correlation between the structural entropy S_{str} [Eq. (3)] and the participation ratio $p = P/N$. For both examples, this behaviour can fairly well be reproduced assuming a decay form

$$|\psi(r)|^2 \;=\; \begin{cases} \exp(-r) & \text{for } r < R \\ C\,[\cos(cr+\phi)+1]\,r^{-2\alpha} & \text{for } r \geq R \end{cases} \tag{6}$$

with $R = 0.75$, $c = 10$, $\alpha = 0.65$ for the Penrose case, and $R = 2.5$, $c = 25$, $\alpha = 0.8$ for the AKN tiling, corresponding to the curves labeled (a) in Fig. 1.

Fig. 2 shows the results of a box-counting multifractal analysis on the eigenstates. The singularity spectra obtained for the Penrose case are almost independent of the size of the systems, and become wider as one moves from the edge to the center of the band. In contrast, the states in the AKN tiling, apart from those close to the band edge, show the behaviour of extended states; the singularity strengths $\alpha(0)$ and $\alpha(1)$ shown in Fig. 2 are very close to 3, hence we cannot conclude a multifractal structure of the states.



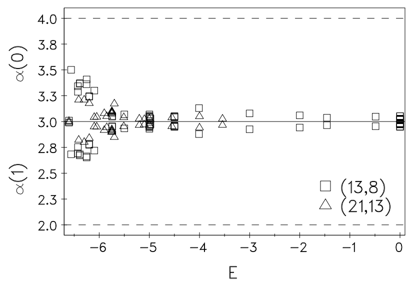


Figure 2: Singularity spectra $f(\alpha)$ and singularity strengths $\alpha(0)$ and $\alpha(1)$ for various eigenstates of periodic approximants of the Penrose (left) and the AKN (right) tiling, respectively.

4 Concluding remarks

Typical eigenstates of a vertex-type tight-binding model on the Penrose tiling have multifractal properties and show a power-law localization. This is in accordance with results on analytically constructed eigenstates.[5]

From our numerical analysis, we cannot draw similar conclusions for the AKN case. While the scaling behaviour of the participation number and the multifractal analysis favour extended states, the structural entropy hints at a power-law decay. In order to answer this question, other quantities have to be investigated which are sensitive also to weak power-law decays. Introducing disorder via the on-site term V_j leads to a localization transition which appears to be very similar to the metal-insulator transition observed in a simple cubic lattice.[6] This corroborates the notion that the eigenstates in the AKN tiling without disorder are extended.

References

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